

Program

PROGRAM SUMMARY

Sunday, 5 th of June 2016	
14:00-19:00	Registration

Monday, 6 th of June 2016		
08:00-09:15	Registration	
09:15-09:25	Opening Addresses	
09:25-09:55	Metrangolo, P.	KN01
09:55-10:20	Rissanen, K.	OC01
10:20-10:45	Legon, A.	OC02
10:45-11:15	Coffee break	
	Fundamentals	
11:15-11:40	Roshoka, S.	OC03
11:40-12:05	Brinck, T.	OC04
12:05-12:30	Kahng, S. J.	OC05
12:30-14:00	Lunch	
	Fundamentals	
14:00-14:25	Pennington, W.	OC06
14:25-14:50	Zeng, Y.	OC07
14:50-15:15	Jindrich, F.	OC08
15:15-15:40	Riedel, S.	OC09
15:40-16:05	Bruce, D. W.	OC10
16:05-16:35	Coffee break	
	Biomedical and biomolecular	
16:35-17:00	Boeckler, F.	OC11
17:00-17:25	Carlsson, A.-C. C.	OC12
17:25-17:50	Poznanski, J.	OC13
17:50-18:20	Groll, M.	KN02

Tuesday, 7th of June 2016

09:00-09:30	Bruce, D. W.	KN03
Fundamentals		
09:30-09:55	Bartashevich, E.	OC14
09:55-10:20	Tsuzuki, S.	OC15
10:20-10:45	Gontrani, L.	OC16
10:45-11:15	<i>Coffee break</i>	
Biomedical and biomolecular		
11:15-11:40	Ho, S. P.	OC17
11:40-12:05	Jindrich, F.	OC18
12:05-12:35	Zhu, W.	KN04
12:35-14:00	<i>Lunch</i>	
14:00-14:30	Shaik, S.	KN05
Fundamentals		
14:30-14:55	Abate, A.	OC19
14:55-15:20	Řezáč, J.	OC20
15:20-15:45	Nakanishi, W.	OC21
15:45-16:15	Esterhuysen, C.	KN06
16:15-16:45	<i>Coffee break</i>	
16:45-21:00	Poster session /City Reception	

Wednesday, 8th of June 2016

09:00-09:30	Beer, P.D.	KN07
Rising Stars Session		
09:30-09:55	Priimagi, A.	RS1
09:55-10:20	Breugst, M.	RS2
10:20-10:45	Berryman, O.	RS3
10:45-11:15	<i>Coffee break</i>	
Young Researchers Session		
11:15-11:40	Karim, A.	YR1
11:40-12:05	Winiewska, M.	YR2
12:05-12:30	D'Agostino, S.	YR3
12:30-14:00	<i>Lunch</i>	
14:00-14:30	Haukka, M.	KN08
Young Researchers Session		
14:30-14:55	Ford, M.	YR4
14:55-15:20	Kurczab, R.	YR5
15:20-15:45	Roseveare, T.	YR6
17:00-22:00	Excursion	

Thursday, 9th of June 2016

09:00-09:30	Ishihara, K.	KN09
Crystal Engineering		
09:30-09:55	Aakeröy, C.	OC22
09:55-10:20	Micallef, A.	OC23
10:20-10:45	McMurtrie, J.	OC24
10:45-11:15	<i>Coffee break</i>	
Crystal Engineering		
11:15-11:40	Đakovic, M.	OC25
11:40-12:05	Catalano, L.	OC26
12:05-12:30	Bryce, D.	KN10
12:30-14:00	<i>Lunch</i>	
12:20-12:50	Li, Z.T.	KN11
Liquid Systems		
14:30-14:55	Schöllhorn, B.	OC27
14:55-15:20	Dumele, O.	OC28
15:20-15:45	Bowling, N.	OC29
15:45-16:10	Huber, S.	OC30
16:10-16:40	<i>Coffee break</i>	
Liquid Systems & Crystal Engineering		
16:40-17:05	Maugeri, L.	OC31
17:05-17:30	Formigue, M.	OC32
17:30-17:55	Jin, W. J.	OC33
17:55-18:25	Goroff, N.	KN12
19:30-22:00	Conference dinner	

Friday, 10th of June 2016

09:00-09:30	Resnati, G.	KN13
Crystal Engineering		
09:30-09:55	Chierotti, M. R.	OC34
09:55-10:20	Clegg, J.	OC35
10:20-10:45	Cinčić, D.	OC36
10:45-11:15	<i>Coffee break</i>	
Applications		
11:15-11:40	Ayzac, V.	OC37
11:40-12:05	Kaiho, T.	OC38
12:05-12:35	Rebek, J. Jr.	KN14
12:35-12:50	<i>Closing remarks</i>	
12:50-14:20	<i>Lunch</i>	

Scientific program

Monday, 6th of June 2016

08:00-09:15

Registration

09:15-09:25

Opening Addresses

Session Chair: Erdelyi, M.

09:25-09:55

Metrangolo, P.

KN1

Halogen Bonding: A New Supramolecular Tool in the Molecular Self-Assembly of Peptides

09:55-10:20

Rissanen, K.

OC01

Very Strong N-X•••O-N Halogen Bonds

10:20-10:45

Legon, A.

OC02

F₂ as a Weak Halogen Bond Donor but the F Atom as a Halogen Bond Strengthener

Fundamentals

Session Chair: Legon, A.

11:15-11:40

Rosokha, S.

OC03

Halogen-bond Assisted Electron and Halogen Transfer

11:40-12:05

Brinck, T.

OC04

Analysis of Halogen Bonding using Local Molecular Surface Properties: Revisiting the Importance of Charge Transfer

12:05-12:30

Kahng, S. J.

OC05

Chiral 2-dimensional Molecular Structures with Halogen Bonds Studied Using Scanning Tunneling Microscopy

Scientific program

Fundamentals

Session Chair: Ho, S.

14:30-14:55	Pennington, W.	OC06
	X-panded Polyiodides and Triiodide×Asymmetry in Organoiodine Hybrid Salts	
14:55-15:20	Zeng, J.	OC07
	Beyond Halogen bonding: Group III σ -hole Interactions and Ylide-containing σ -hole Interactions	
15:20-15:45	Jindrich, F.	OC08
	σ -Hole Interactions of Boron Clusters	
15:45-16:10	Riedel, S.	OC09
	Polyhalogen Anions: Examples for Halogen-Halogen Bonding	
16:10-16:35	Bruce, D. W.	OC10
	What do we Learn about Halogen Bonding from the Study of Liquid Crystals and Related Systems?	

Biomedical and biomolecular

Session Chair: Esterhuysen, C.

17:05-17:30	Boeckler, F.	OC11
	Opportunities and Limitations for Halogen Bonds in Molecular Design	
17:30-17:55	Carlsson, A.-C. C.	OC12
	Engineering Halogen Bonds to Affect Protein Stabilization	
17:55-18:20	Poznanski, J.	OC13
	Competition between Halogen Bonding and Electrostatic Interactions Identified in Complexes of Protein Kinase CK2 α with Halogenated Ligands	
18:20-18:45	Groll, M.	KN02
	Halogens and their Prerequisites for Protein:Ligand Interactions	

Scientific program

Tuesday, 7th of June 2016

Session Chair: Huber, S.

09:00-09:30 Bruce, D. W. **KN03**
Molecular Analogues of *In Vivo* Halogen-bonding Situations

Fundamentals

09:30-09:55 Bartashevich, E. **OC14**
Targeting the Iodine Halogen Bond: The Role of C-I Covalent Interactions

09:55-10:20 Tsuzuki, S. **OC15**
Origin of Attraction and Directionality of Halogen Bond and Chalcogen Bond

10:20-10:45 Gontrani, L. **OC16**
X-Rays and Molecular Dynamics Reveal Halogen Bond in Liquid Acetonitriles

Biomedical and biomolecular

Session Chair: Rissanen, K.

11:15-11:40 Ho, Shing P. **OC17**
Biological Halogen Bonds

11:40-12:05 Jindrich, F. **OC18**
The Effect of Halogen-to-Hydrogen Bond Substitution on Human Aldose Reductase Inhibition

12:05-12:35 Zhu, W. **KN04**
Computational Study and Application of Halogen Bonding between Drug and Target Protein

14:00-14:30 Shaik, S. **KN05**
On The Nature of the Halogen Bond

Scientific program

Fundamentals

Session Chair: Metrangolo, P.

14:30-14:55	Abate, A. Halogen-Bond Driven Self-Assembly of Perfluorocarbon Monolayers	OC19
14:55-15:20	Řezáč, J. Quantification Of Charge Transfer Contribution To Energetics Of Halogen Bonding	OC20
15:20-15:45	Nakanishi, W. Behavior of Extended Hypervalent $\sigma(4c-6e)$ Interactions Containing Halogen Atoms, Elucidated with QTAIM Dual Functional Analysis	OC21
15:45-16:15	Esterhuysen, C. Gold as Lewis base	KN06
16:45-21:00	Poster session	

Scientific program

Wednesday, 8th of June 2016

Session Chair: Pennington, W.

09:00-09:30 Beer, P.D. **KN07**
Halogen Bonding Interlocked Host Molecules for Anion Recognition and Sensing

Rising Stars Session

09:30-09:55 Priimagi, A. **RS1**
Towards Halogen-Bonded Photoactuators: A Glimpse into the Future

09:55-10:20 Breugst, M. **RS2**
Mechanisms of Molecular-Iodine-Catalyzed Reactions

10:20-10:45 Berryman, O. **RS3**
A Halogen Bond Induced Triple Helicate Encapsulates Iodide

Young Researchers Session

Session Chair: Esterhuysen, C.

11:15-11:40 Karim, A. **YR1**
Counterion Influence on the N-I-N Halogen Bond

11:40-12:05 Winiewska, M. **YR2**
Thermodynamic Study on Binding of Halogenated Ligands by PK CK2 Reveals Dominance of Electrostatic Interactions Over Halogen Bonding

12:05-12:30 D'Agostino, S. **YR3**
Fluorescent and Phosphorescent Co-Crystals Based on Halogen Bonds

14:00-14:30 Haukka, M. **KN08**
Halogen Bond Donors: Dihalogens

Scientific program

Young Researchers Session

Session Chair: Huber, S.

14:30-14:55	Ford, M.	YR4
	X-TINKER: A Computational Algorithm for the Rational Design of Biological Halogen Bonding	
14:55-15:20	Kurczab, R.	YR5
	Halogen Bonding - the Role and Significance in Interactions of Ligands with Class A GPCRs	
15:20-15:45	Roseveare, T.	YR6
	Using Halogen Bonding to Control Pore Space	

Scientific program

Thursday, 9th of June 2016

Session Chair: Metrangolo, P.

09:00-09:30	Ishihara, K.	KN09
	Cooperative Activation with Chiral Lewis Base Catalysts and <i>N</i> -Haloimides: Catalytic Enantioselective Iodocyclization	

Crystal Engineering

09:30-09:55	Aakeröy, C.	OC22
	Halogen Bonds from Fundamentals to Applications	

09:55-10:20	Micallef, A.	OC23
	Halogen Bonding in the Assembly of Nitroxide Based Materials	

10:20-10:45	McMurtrie, J.	OC24
	Manipulation of Spin Crossover in Metal Complexes Encapsulated in Halogen Bond Networks	

Crystal Engineering

Session Chair: Resnati, G.

11:15-11:40	Đakovic, M.	OC25
	Halogen Bonding Interaction in Assemblies of Metal Complexes: Resemblance to Hydrogen Bond	

11:40-12:05	Catalano, L.	OC26
	Highly Efficient Rotational Dynamics in Supramolecular Rotors Assembled through Halogen-Bonding	

12:05-12:30	Bryce, D.	KN10
	Solid-State NMR Studies of Sigma-Hole Interactions	

12:20-12:50	Li, Z. T.	KN11
	Halogen Bonding and Conjugated Radical Cation Dimerization in Solution	

Scientific program

Liquid Systems

Session Chair: Ho, S.

14:30-14:55	Schöllhorn, B.	OC27
	Electrochemical Switching of Halogen Bonding in Solution	
14:55-15:20	Dumele, O.	OC28
	Halogen Bonding Supramolecular Capsules for the Quantification of Weak XB in Solution	
15:20-15:45	Bowling, N.	OC29
	Halogen Bonding in the Design of Conjugated Organic Molecules	
15:45-16:10	Huber, S.	OC30
	Multidentate Halogen Bonding Organocatalysts in Molecular Recognition Studies	

Liquid Systems & Crystal Engineering

Session Chair: Legon, A.

16:40-17:05	Maugeri, L.	OC31
	Neutral Iodotriazoles as Scaffolds for Stable Halogen-Bonded Assemblies in Solution	
17:05-17:30	Formigue, M.	OC32
	Cocrystal or Salt: Solid State-Controlled Iodine Shift in Crystalline XB Systems	
17:30-17:55	Jin, W. J.	OC33
	Tunable Colors of Organic Cocrystal Phosphores by Halogen Bond	
17:55-18:25	Goroff, N.	KN12
	Halogen-Bond-Controlled Assembly of Halodiyne for Topochemical Polymerization to Make Linear and Ladder Conjugated Polymers	

Scientific program

Friday, 10th of June 2016

Session Chair: Rissanen, K.

09:00-09:30 Resnati, G. **KN13**
Halogen Bond and Beyond

Crystal Engineering

09:30-09:55 Chierotti, M. R. **OC34**
New Insights on the Characterization of Halogen Bond by
Means of Solid-State NMR

09:55-10:20 Clegg, J. **OC35**
Reticular Design of Three-Dimension Halogen Bonding
Frameworks Employing Metallo-ligand Nodes

10:20-10:45 Cinčić, D. **OC36**
Halogen Bonding of *N*-Bromophthalimide via Grinding and
Solution Crystallization

Applications

Session Chair: Pennington, W.

11:15-11:40 Ayzac, V. **OC37**
A Supramolecular Tool To Measure Halogen-Halogen
Interactions In Solution

11:40-12:05 Kaiho, T. **OC38**
Industrial Applications of Halogen Bonding

12:05-12:35 Rebek, J. Jr. **KN14**
Molecular Behavior in Small Spaces

12:35-12:50 *Closing remarks*

Poster session

Tuesday, 7th of June 2016

- P01** Li, C.; Jin, W. J.
Halogen Bond Adsorption Isotherms of Iodo-perfluorobenzenes on Strong anion Exchange Sorbents
- P02** Engelage, E.; Schulz, N.; Linke, A.; Jungbauer, S. H.; Huber, S.; Waldvogel, S. R.
Potent Affinity Material For Tracing Acetone And Related Analytes Based On Molecular Recognition By Halogen Bonds
- P03** Jiang, S.; Shang, H.; Wang, Y.; Wang, Y.
Halogen Bonding Complexes based on Azopyridines: Liquid Crystallinity and Photoresponsive Properties
- P04** Wang, Y.; Wei, J.; Jiang, S.
Br...Br Bonding Interaction Based Crystalline Matrix Induced Temperature Phosphorescence of Organic Molecules
- P05** Schulz, N.; Bulfield, D.; Jungbauer, S. H.; Walter, S. M.-; Schindler, S.; Rout, L.; Kniep, F.; Huber, S. M.
A Halogen Bonding Catalyzed Diels-Alder Reaction
- P06** Gliese, J. P.; Dreger, A.; Jungbauer, S. H.; Huber, S. M.
Cationic Multidentate Halogen-Bond Donors in Halide Abstraction Organocatalysis: Catalyst Optimization by Preorganization
- P07** Siiskonen, A.; Priimagi, A.
Comparison of Small Basis Set on Describing Halogen Bonding
- P08** Riedel, S.; Müller, C.; Brückner, R.; Haller, H.; Sonnenberg, K.
Theoretical Investigations of Periodic Polyhalogen Networks
- P09** Kumar, V.; Pilati, T.; Quici, S.; Meytrangelo, P.; Resnati, P.
Halogen Bonded Adducts Involving HCCrypt-111 Iodide Helps in Exploring Hydrogen Bonding Features
- P10** Takeda, Y.; Hatanaka, K.; Minakata, S.
Self-Complementary Two- and Four-point Halogen Bonding (XB) Motifs in 1,3-Dibromothieno[3,4-c]heterole-4,6-diones
- P11** Valkonen, A.; Rissanen, K.
Trisubstituted Mesitylene Core Based Tridendate Halogen Bond Donors
- P12** Xu, Y.; Viger-Gravel, J.; Korobkov, I.; Bryce, D. L.
A Combined Solid-State Multinuclear Magnetic Resonance and Molecular Orbital Study of P=O...I-C Halogen Bonding

- P13** Wang, H.; Chen, L.; Zhang, D. W.; Li, Z. T.
Protonation-induced Switching of Pleated Foldamers of Diaminonaphthalene-bipyridinium Alternating Dynamic Covalent Polymers
- P14** Meng, L. P.; Mo, L. X.; Zeng, Y. L.; Li, X. Y.
Halogen Bond and Chalcogen Bond in Complexes Involving SX₂ (X = F, Cl, and Br)
- P15** Rowe, R. K.; Ho, P. S.
Engineering Halogen Bonds as a Novel Protein-Protein Interaction
- P16** Danelius, E.; Andersson, H.; Lood, K.; Jarvoll, P.; Brath, U.; Erdelyi, M.
Studies of Weak Interactions in Solution Using a Dual β -Hairpin Model System
- P17** Para, R. D.
Proton and Iodonium Ion Transfer in the Mixed Dimer of Formamidine and *N*-Iodinated Formamidine: an ab initio Study
- P18** Riwar, L.-J.; Harder, M.; Trapp, N.; Diedrich, F.
Investigating the Nature of π Stacking — Development of Rebek Imide-Type Model Systems
- P19** Zhang, X. Y.; Wang, Y. H.; Zeng, Y. L.; Li, X. Y.; Meng, L. P.
The Mutual Influence Between π -Hole Pnictogen Bonds and σ -Hole Halogen Bonds in Complexes of PO₂Cl and XCN/C₆H₆ (X = F, Cl, Br)
- P20** Gottschalk, H. C.; Suhm, M. A.
Control over the Hydrogen Bond Docking Site in Anisole by Ring Alkylation and Halogenation
- P21** Jabłoński, M.
IMCIHB vs M \cdots (H-Si) Agostic Bonds and M \cdots (η^2 -SiH) σ Interactions
- P22** Dreger, A.; Gliese, J.-P.; Jungbauer, S. H.; Schindler, S.; Herdtweck, E.; Keller, S.; Huber, S. M.
Multiple Multidentate Halogen Bonding in Solution, in the Solid State, and in the (Calculated) Gas Phase
- P23** Geboes, Y.; De Proft, F.; Herrebout, W. A.
Halogen Bonding versus Lone Pair \cdots π -interactions: Competitive Noncovalent Interactions with Perhalogenated Alkenes
- P24** Turunen, L.; Warzok, U.; Puttreddy, R.; Schalley, C. A.; Rissanen, K.
Capsular Assemblies Through Halonium Ions
- P25** Southern, S.; Errulat, D.; Frost, J.; Bryce, D. L.
Solid-State NMR Investigations of Tetrel Bonds
- P26** Hayashi, S.; Sugibayashi, Y.; Nakanishi, W.
Halogen Bonds of the $n \rightarrow \sigma^*$ Type versus Conventional Hydrogen Bonds: Behavior of the XB and HB Interactions Elucidated with QTAIM-DFA
- P27** Tepper, R.; Schulze, B.; Görls, H.; Bellstedt, P.; Jäger, M.; Schubert, U. S.
Preorganization In A Cleft-Type Anion Receptor Featuring Iodo-1,2,3-Triazoles As Halogen Bond Donors

- P28** Bulfield, D.; Engelage, E.; Jungbauer, S.H.; Kniep, F.; Lehmann, C.; Herdtweck, E.; Huber, S. M.
Toward Molecular Recognition: Three-Point Halogen Bonding in Solid State and Solution
- P29** Fave, C.; Olivera, R.; Groni, S.; Branca, M.; Mavré, F.; Lorcy, D.; Formigué, M.; Schöllhorn, B.
Electrochemical Activation of a Tetrathiafulvalene Based Halogen Bond Donor for Anion
Recognition in Polar Solvents.
- P30** Salunke, J. K.; Sacone, M.; Terraneo, G.; Cavallo, G.; Metrangolo, P.; Primagi, A.
Design, Synthesis, Optical and Electrochemical Properties of Carbazole-based Halogen-
Bonded Organic Semiconductors
- P31** Ciesielski, W.
Halogenated Carbon Nanotubes Functionalized By Salts Containing Stereogenic Heteroatoms
As Electrodes In Their Battery Cells